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Molecular dynamics simulation of fatigue damage in metals

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THESIS

MOLECULAR DYNAMICS SIMULATION OF FATIGUE DAMAGE IN METALS

by

William S. Lunt

December 2003

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MOLECULAR DYNAMICS SIMULATION OF FATIGUE DAMAGE IN METALS

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Submitted in partial fulfillment of the
requirements for the degree of

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ABSTRACT

Molecular dynamics simulation was conducted to better understand the mechanism of fatigue failure and to identify a parameter(s) that can indicate progressive damage due to cyclic loading. The Embedded Atom Method (EAM) was used for copper atoms subjected to cyclic loadings. Defective crystal structures including vacancies or impurities were considered for the study. The results showed that there was an increase in potential energy and kinetic energy, respectively, in the metal as the number of cycles increased. This means the metal becomes weaker, i.e., an indication of progressive damage. Therefore, the change of potential energy may be used as an indicator for fatigue damage accumulation. Furthermore, the relative distances between vacancies (or impurities) increased globally with fluctuation as the number of loading-unloading cycles increased.

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I. INTRODUCTION

A. MOTIVATION

Molecular dynamics simulation of metallic atoms under conditions of cyclic loading may provide beneficial insight to the problem of fatigue failure. As the number one cause of metallic failure and its inherent unpredictability, fatigue warrants in depth research [1]. In materials possessing defects, fatigue has been shown to occur at the location of defects and sometimes far below the elastic limit. A greater understanding of the mechanism of fatigue and of the behavior of defects under a number of cycles may allow the prediction of behavior at a high number of cycles leading to a more exact prediction of the number of cycles before fatigue failure occurs.

B. BACKGROUND

Much of our understanding of material properties on the macroscopic level comes from empirical data rather than an understanding of atomic interactions resulting in the properties. Designs accounting for fatigue have proven to be time consuming and expensive. Molecular dynamics simulation is giving a clearer understanding of the relation between atomic interaction and its effect on the macroscopic level.

Additionally, advances in nanotechnology have led to the production of nanoscale devices and fatigue failure in those devices is a problem that must be addressed [2].

The property associated with material failure due to cyclic loading is known as the fatigue strength in materials and is an example of a property that is based on empirical data.

Fatigue is a damage-accumulation process of real materials under cyclic loads. Defects such as impurities and vacancies play an important role in fatigue. When a material including those defects is stressed even in the elastic range, there are irreversible changes within the material, which are initially so small that such changes are not measurable in the stress-strain curve. However, as the number of cycles in the loads increases significantly, those changes lead to ultimate failure of the materials [3].

The purpose of this research is to understand the mechanism of fatigue damage in metallic materials that may ultimately result in a more accurate prediction of cycles to failure. Empirical data shows that metal under cyclic loading will fail earlier in material with defects and that failure will occur in the vicinity of the defects [3]. Inherent defects in material and their behavior under cyclic loading may provide valuable insight into when and where failure will occur. Molecular dynamics simulation using the embedded atom method was used in this study to research the behavior of the defects and the overall response of the system in terms of potential and kinetic energy.

C. PREVIOUS RESEARCH

Chang and his coworker [4,5] studied the behavior of copper under tensile and fatigue conditions through the use of molecular dynamics simulation. They used a Lennard-

Jones potential model and developed stress vs. strain curves for both varying percentages of vacancies, and varying temperatures. The results of their research showed that increasing the number of vacancies resulted in lower stress strain curves and increasing the temperature resulted in a decreased Young's modulus. In addition, they also studied stress versus the number of cycles to failure for both varying vacancy percentages and varying temperatures. They found that lower vacancy percentages and higher temperatures resulted in a higher fatigue strength.

Yasukawa [6] studied the influence of moisture on the static-fatigue strength of silicon oxide using the extended Tersoff inter-atomic potential. The potential considered inter-atomic charge transfers between atoms of different species during the process of their reaction. In this study, the author explained the mechanism of strength decrease of silicon oxide due to moisture.

Ye, Farkas, and Soboyejo [7] studied fracture toughness and fatigue crack growth experimentally and theoretically. They used the embedded atom method [8,9] for the theoretical study, which was used to explain some experimental findings. In this study, they focused on understanding the reasons for improved toughness of 40Ti alloy with an incrementally increasing load, but not a cyclic load.

While the preceding studies focused on crack behavior, the objective of this study was to investigate the fatigue process and to identify parameter(s) that could be correlated to progressive damage. The parameter(s) could be used to estimate the expended fatigue life.

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I. ANALYSIS

A. THE EMBEDDED ATOM METHOD

Molecular dynamics simulation using the Paradyn model [10] is the cornerstone of this research. It is important to distinguish the difference between a simulation and a model and its effect on the interpretation of results. In this molecular dynamics simulation, a simulation was performed on a model of copper atoms, not on the actual copper atoms. A model is usually a simplification of a real system that allows targeted study of specific phenomenon. The simplification creates limitations. For example, while the model works in 1-D, it may not work in 2-D [11]. In other words, one must consider the limitations of the selected model when analyzing the results.

In the case of the Paradyn model [10], atoms are treated as point masses with inter-atomic potentials obtained from the embedded atom method [8,9].

The embedded atom method describes the total energy of a system of metallic atoms.

$$E_{tot} = \sum_{i} E_{ee}\left(r_{h,i}\right) + \frac{1}{2}\sum_{i,j} f_{ij}\left(r_{ij}\right) \qquad (1)$$

Equation (1) states that the total energy of the system of atoms is the sum of the embedding energy and the core-core repulsions.

Specifically, the embedding energy term treats each atom, i, as an impurity and is a calculation of the amount of energy required to embed atom i into the electron

density of its actual location. The electron density of its actual location is determined by

$$r_{h,i} = \sum_{j \neq i} r_j^a(r_{ij}) \qquad (2)$$

Equation (2) states that the electron density at the position of atom i is a sum of the densities contributed by all other atoms in the sample within a given distance, r_{ij}. Atoms beyond r_{ij} have no effect on atom i.

The core-core repulsion term in equation (1) is a calculation of the core-core repulsions (f_{ij}) of each atom, i, paired with all other atoms in the sample within a given distance, r_{ij}. Similar to the electron density, atoms beyond a r_{ij} have no core-core repulsion with atom i. The ½ is necessary to avoid counting the same repulsion two times during summation over the entire sample.

In R.A. Duff's thesis, [12], he concluded that Paradyn [10] accurately modeled the modulus of elasticity and stress vs. strain curves of copper when compared with properties determined from empirical methods.

B. MODELING

The model used during this research, entitled Paradyn [10], was written by S. J. Plimpton and B. A. Hendrickson and was based on the code Dynamo, written by S.M. Foiles and M.S. Daw. Dynamo was written to use the embedded atom method in molecular dynamics simulation [8,9].

In general terms, Paradyn receives user inputs that include an atom position file, an atom velocity file, and an inter-atomic potential file.

The position file assigns an identification number (1 to 500 in this study), and Cartesian coordinates to each

atom in units of Angstroms. The final array of atoms is in the shape of a cube or a box. The velocity file assigns a random three-dimensional velocity, in units of Angstroms/picosecond to each atom and a number that corresponds to the same identification number in the position file.

The potential input file assigns parameters determined from the embedded atom method and includes the atomic number, atomic mass, lattice spacing, potential cutoff range for each atom, grid of inter-atomic force, grid of atom electron density and the spherically averaged atomic density [9,12].

Additionally, the user controls an initialization file that directs where to read the initial positions, velocities, and potentials and where to write the final data. It also allows adjustment of boundary conditions and the dimensions of the box containing the array. In this study, periodic boundary conditions were selected so that atoms moving outside of the box boundary would be remapped to the other side of the box. In addition the user can specify applied pressure in units of bar which was used in this study to simulate a cyclic load. The user can also specify the length of the time-steps and the number of time-steps.

Molecular dynamics simulation requires the completion of initialization, equilibration, and production. The description to this point has explained initialization.

Because the system is initialized with random velocities assigned to the atoms, it takes time for the system to reach equilibrium. Analysis of the output data

shows that values such as total energy fluctuate as a result of the random velocities before reaching a constant value. During this research, equilibrium occurred consistently around 1400 time-steps. This begins the production phase and data produced during this period is used in the analysis.

After completion of the simulation, the final data describing the system of atoms is contained in an output log file. The data contained in the log file relevant to this research includes the simulation time in units of picoseconds, the total, potential and kinetic energy in units of electron-volts, the temperature in units of Kelvin, the pressure in units of bar, and the volume of the final sample in cubic angstroms. Additional output files include final positions and final velocities that were then used as inputs for the next load or unload period.

A model of 500 copper atoms arranged in a face-centered cubic array was implemented to investigate the behavior of copper under conditions of cyclic loading. From the original 500-atom model, configurations were created that contained defects in the form of vacancies or impurities. At least two entire rows of atoms were removed to create the configuration containing vacancies. This assisted in visualization of the movement of the vacancies relative to one another. In order to create the configuration with impurities, the vacancies of the previous configuration were replaced with nickel atoms and assigned corresponding potentials.

The simulation was performed on these configurations of atom models to simulate cyclic loading by applying a pressure of 10 bar for a time step of 0.005 psec with a

duration of 1 psec followed by 0 bar applied for the same length of time. This gave a load cycle of 2 psec.

The positions of the defects and the energy data were tabulated at the end of each period of loading and unloading. The positions of the impurities were tracked by recording the coordinates given in the output position file. The positions of the vacancies were tracked by using the average position value of the nearest neighbors in the z direction and were obtained from the output position file.

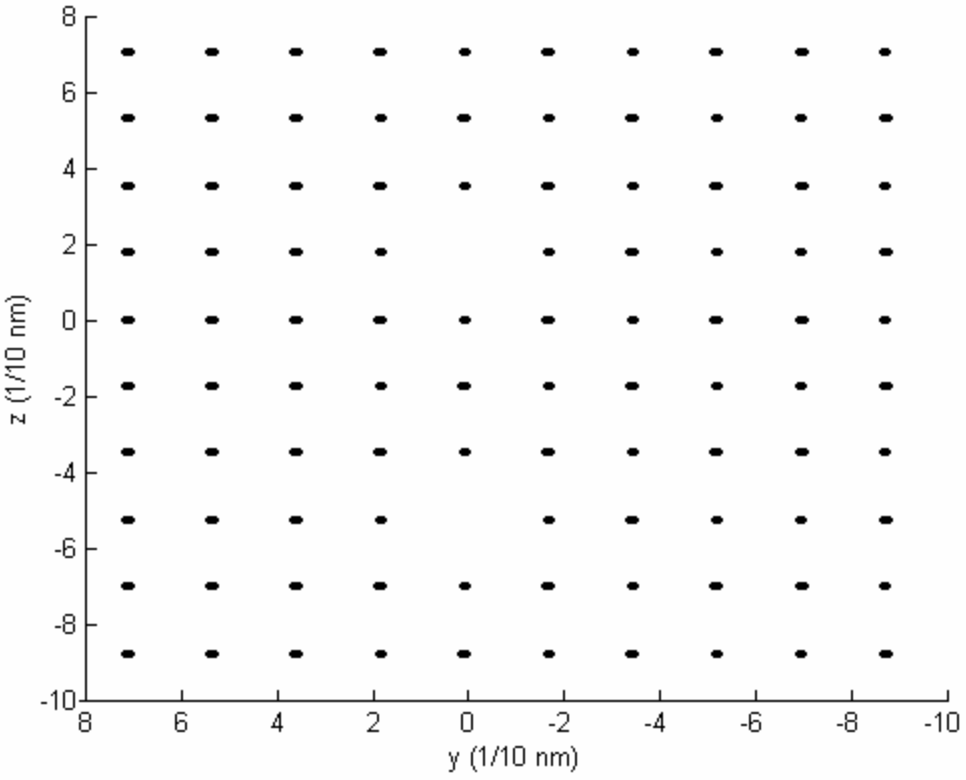

Figure 1. Two-dimensional view of 3-D copper atoms with two rows of vacancies.

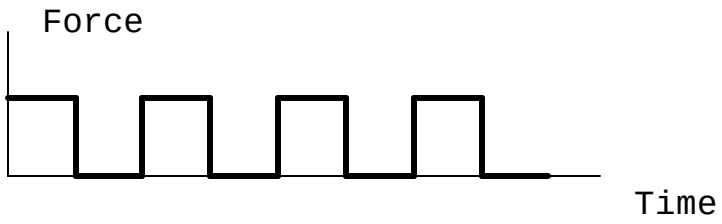

Figure 2. Cyclic loads

III. RESULTS AND DISCUSSION

A. VACANCIES

Figure (3) shows the relative distance between defects vs. the number of cycles. The ones labeled as loaded state represent the positions for each load period. In other words, it shows the position every 2 psec starting with the first load. The figures also compare a parallel load vs. a normal load. A parallel load indicates a load applied along the z-axis of figure (1). It is parallel to the line connecting the vacant positions. A normal load indicates a load applied along the y-axis of figure (1). The load is normal to the line connecting the vacant positions. The figures show a fluctuation of distances with increasing numbers of cycles. The general trend is a separation of the vacancies. The separation of the vacant positions is larger for the parallel load than for the normal load as the number of cycles increases.

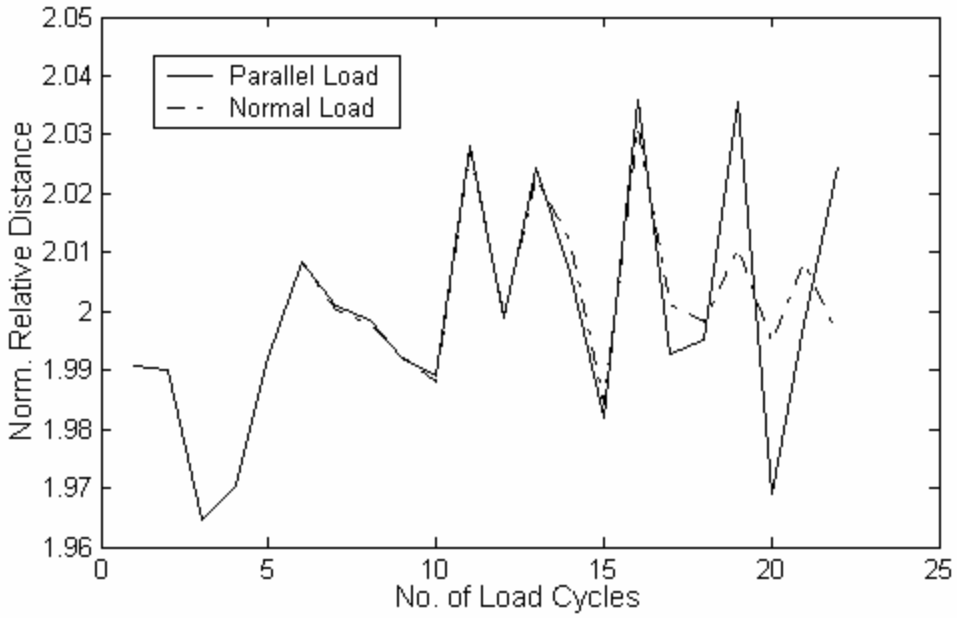

Figure 3. Plot of the normalized distance between the two vacancies vs. the number of cyclic loads at the unloaded state

Figure (4) compares the change in average potential energy of the two loading types. There is an increase in potential energy in both cases as the number of cycles increase. This indicates that as the atoms move apart the progressive strength reduces along with increased cycles. Thus, the potential energy can be an indicator of fatigue damage accumulation. At the same time, there is an increase in the average kinetic energy with increasing cycles. There is only a minor difference in the energy plots for the two loading orientations indicating that whether parallel or normal is irrelevant.

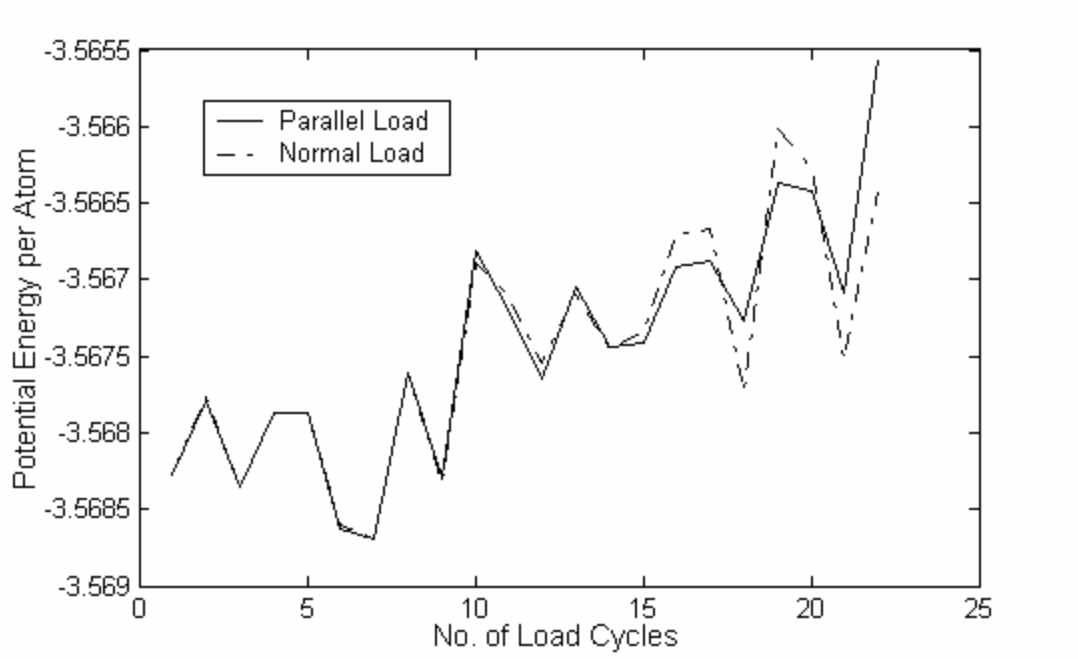

Figure 4. Plot of average potential energy per atom in the system with vacancies vs. the number of cyclic loads at the unloaded state

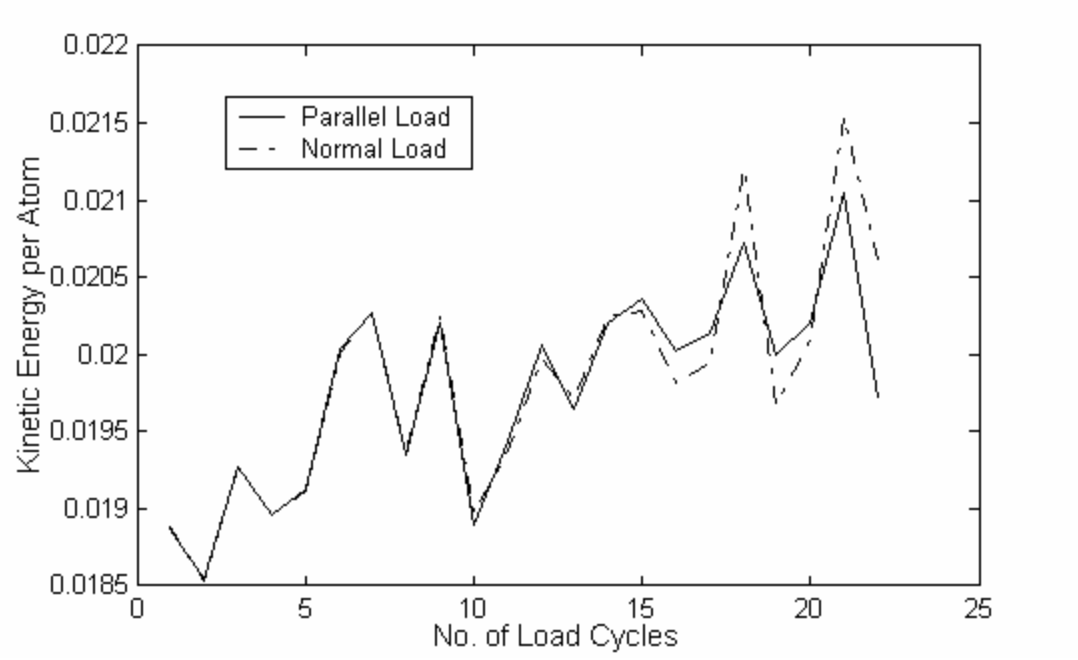

Figure 5. Plot of average kinetic energy per atom in the system with vacancies vs. the number of cyclic loads at the unloaded state

The molecular dynamics model can be considered as a system of masses (atoms) and non-linear springs (inter-atomic forces).

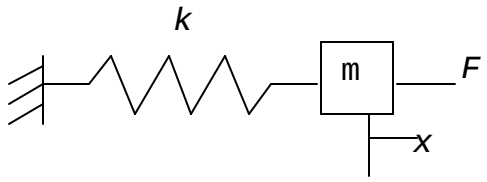

Figure 6. One-dimensional linear spring-mass system subjected to a force

In order to understand the observations taken from the energy plots, let us consider a simple 1-D mass-spring system with a load, as shown in figure (6). The system is assumed to be linear with the mass=1 and the spring constant $k=\pi^2$ so that the natural frequency, ω, is π for simplicity. The mass is subjected to a force F.

When a cyclic load, shown in figure (2), is applied to a system, the energy in the system will vary depending on the timing of the applied force. For example, when the applied force is in the same direction of the motion of the mass, it will produce positive work on the system, i.e. it will increase the energy of the system. Conversely, if the applied force is in the opposite direction of motion, it will reduce the energy of the system. The most dominant energy change is when the frequency of the applied cyclic load is near or equal to a natural frequency of the system. In this case, there is a significant energy increase in the system. Figures (7) and (8) illustrate this.

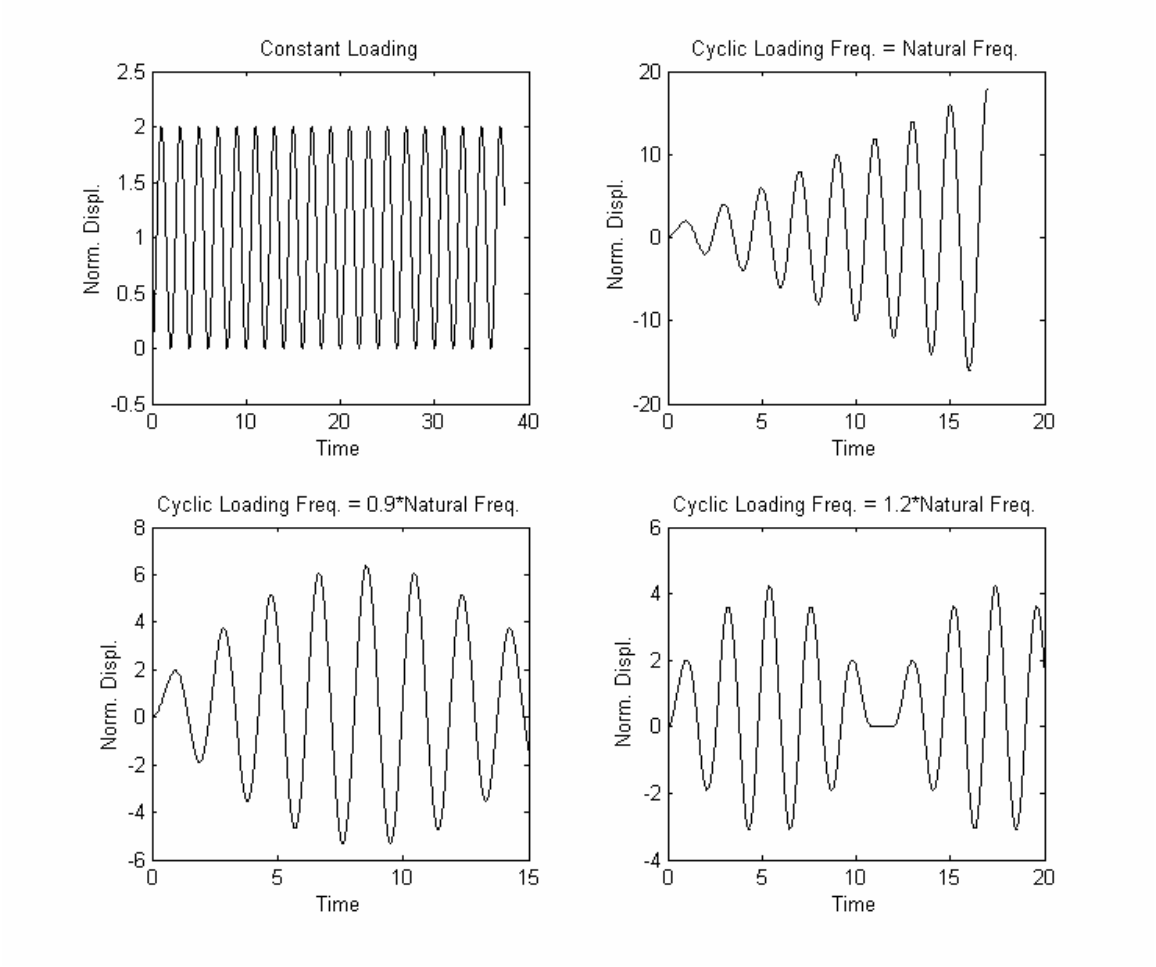

Figure 7. Normalized displacement plots of a spring-mass system with cyclic loads of different frequencies and the same magnitude

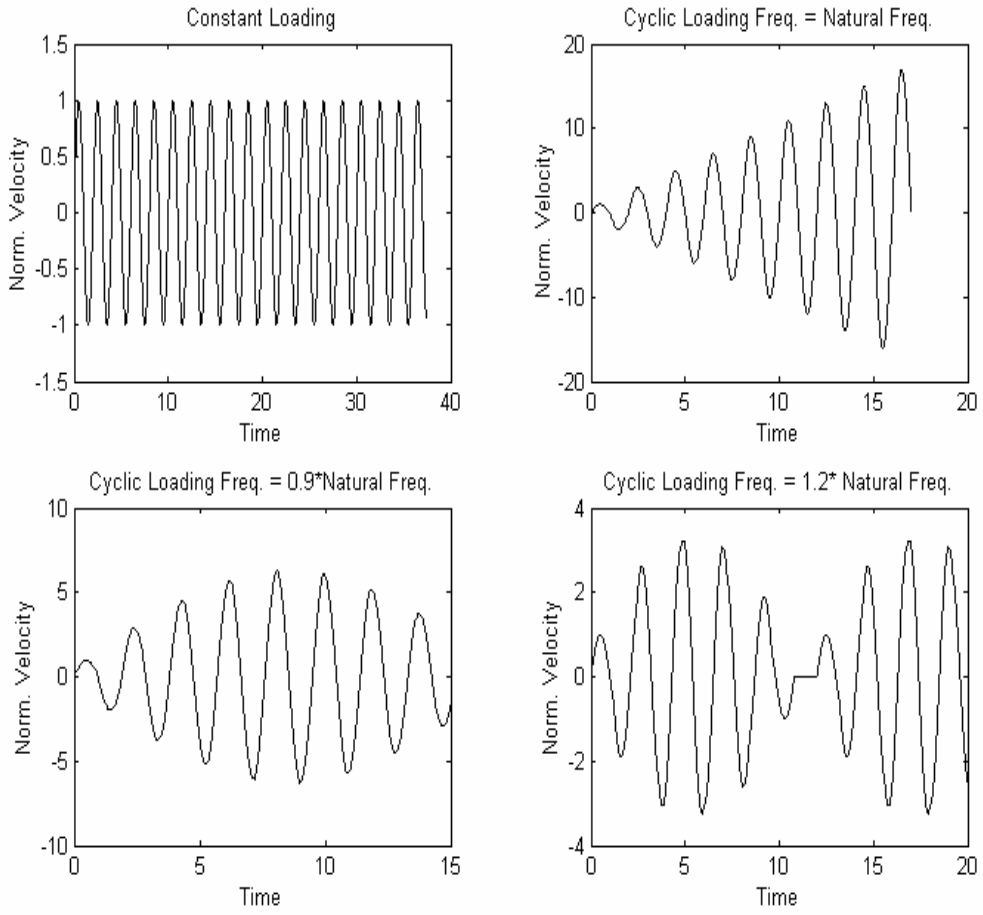

Figure 8. Velocity plots of a spring-mass system with cyclic loads of different frequencies and the same magnitude

In the first case, the force is constant, no cyclic loading. Then the top left plots in figures (7) and (8) show the normalized displacement and velocity of the mass along with time. The displacement was normalized with respect to the static displacement of the spring, F/k, while the velocity was normalized with respect to F*ω/k.

The other three plots in both figures are for cyclic loads as sketched in figure (2). In each case the cyclic loading frequency is different. The top right plots are the case of resonance. The bottom two plots in both figures are for the cyclic loadings whose frequencies are near the natural frequency of the 1-D spring-mass system. As shown in the figures, both displacement and velocity increase significantly near the natural frequency.

In representation of the molecular dynamics model by masses and springs, there are a large number of natural frequencies in a large range whose number is equal to the number of degrees of freedom. As a cyclic load is applied to the system, the frequency of the load is very likely close to one of the natural frequencies. Then, there is a significant rise of displacement and velocity, which contributes to the increase of potential and kinetic energy of the system, respectively as shown in figures (4) and (5).

B. IMPURITIES

The next case studied the inclusion of impurities. The positions of vacancies of the previous case were replaced with nickel atoms. Then the same cyclic loading was applied. Figure (9) shows the relative displacements between two impure atoms. There is a slow trend with a large fluctuation of the two impure atoms moving away from each other as the number of cycles increase. There is little difference between the two different loading orientations. However, the increase of average potential energy per atom (Figure (10)), and increase of the average kinetic energy (figure (11)) are very similar to those with vacancies (figures (4) and (5), respectively).

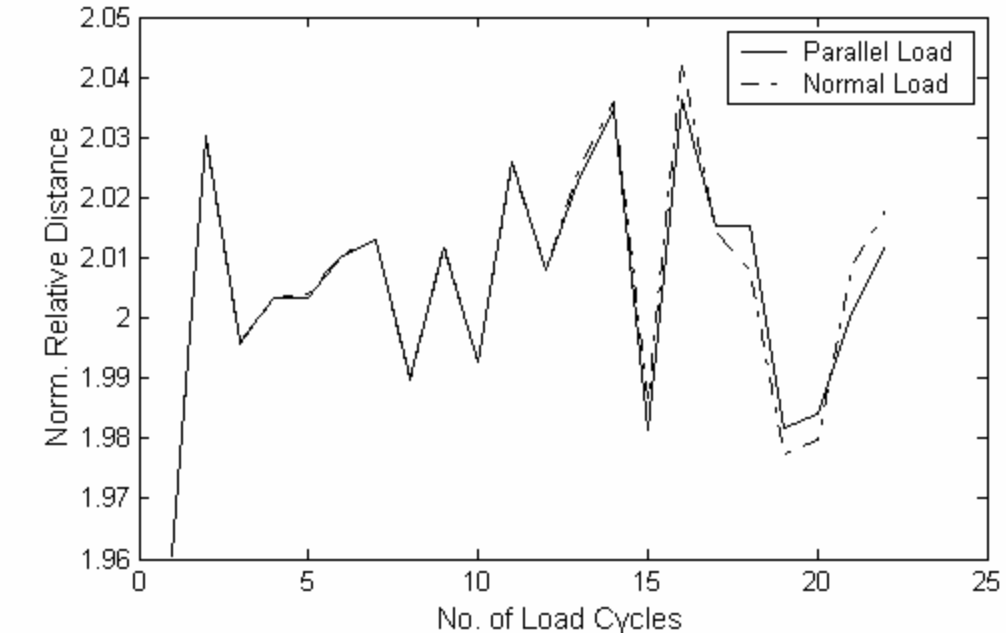

Figure 9. Plot of the normalized distance between the two impurities vs. the number of cyclic loads at the unloaded state

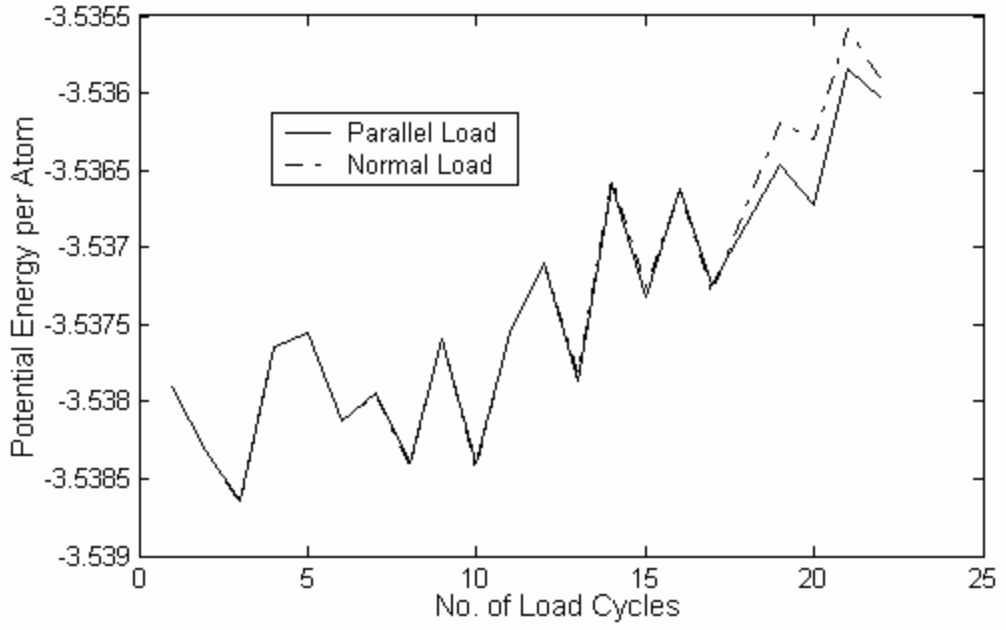

Figure 10. Plot of average potential energy per atom in the system with impurities vs. the number of cyclic loads at the unloaded state

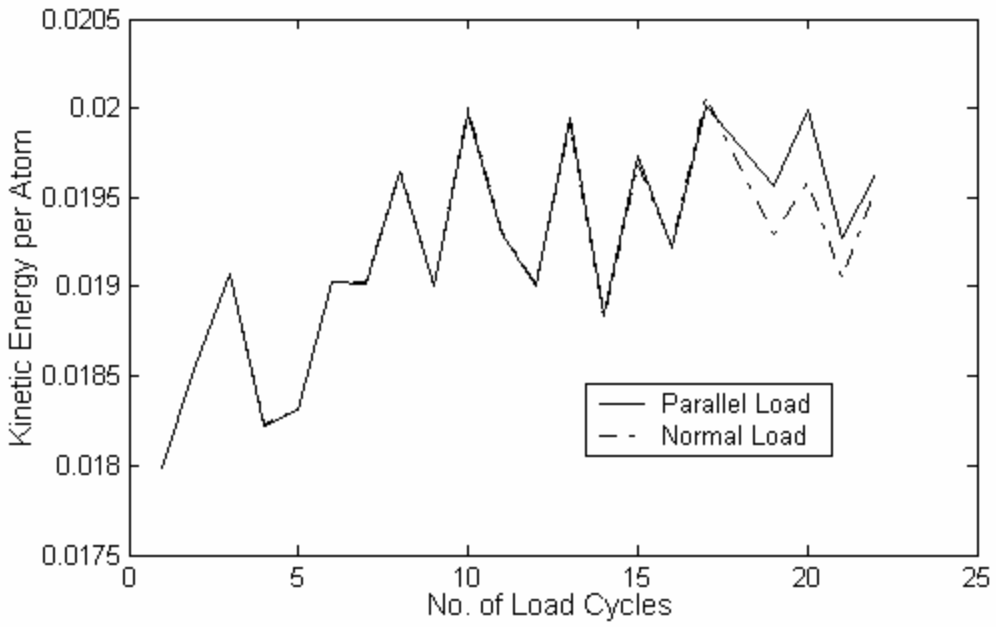

Figure 11. Plot of average kinetic energy per atom in the system with impurities vs. the number of cyclic loads at the unloaded state

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IV. CONCLUSIONS AND RECOMMENDATIONS

Molecular dynamics simulation was conducted to understand the fatigue damage process in pure copper. Both vacancies and impurities were considered in the model with two different orientations of cyclic loads. The results showed that the relative distance between the vacancies or the impurities, respectively, increased along with the increasing number of cycles. This indicated overall separations among atoms as the cyclic load continued. The statement was also supported when the average potential energy per atom was plotted against the number of cyclic loads. There was an increase in the potential energy and kinetic energy, respectively, with some fluctuation as the number of load cycles increased. This also meant an increase of the total energy with cyclic loads. Those results implied the weakening of the material, i.e., fatigue damage, caused by the cyclic load. The orientation of loadings with respect to either vacant positions or impure atoms was insignificant in fatigue damage. Finally, and explanation for the increase of energy in a system with a cyclic load was provided using a 1-D spring-mass model.

The following are recommended for further study:

1. Compare the results of this study with other metallic materials containing similar defect configurations.

2. Compare the results of this study with different cases of applied cyclic loading and determine whether a different trend occurs with different applied loads.

3. Increase the loading cycle to be less than, but near the fatigue strength of copper and compare the results with a loading cycle exceeding the fatigue strength.

4. Run the simulation with a larger number of cycles and perform a trend analysis to predict fatigue life cycles of materials.

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